### Black box variational Bayes

"Black box variational Bayes" (BBVI) is a set of techniques for quickly and automatically approximating Bayesian posteriors using optimization. I'll consider "mean field automatic differentiation variational inference" (ADVI).

### Black box variational Bayes

"Black box variational Bayes" (BBVI) is a set of techniques for quickly and automatically approximating Bayesian posteriors using optimization. I'll consider "mean field automatic differentiation variational inference" (ADVI).

Let  $\theta$  denote model parameters and y some data and the joint generating distribution be  $\mathbb{P}\left(\theta,y\right)=\mathbb{P}\left(y|\theta\right)\mathbb{P}\left(\theta\right)$ . Let  $\mathbb{Q}\left(\theta|\eta\right)$  be a family of candidate approximate posteriors, here taken to be independent normals.

ADVI aims to find

$$\overset{*}{\eta} := \operatorname*{argmin}_{\eta} \operatorname{KL}\left(\mathbb{Q}\left(\theta | \eta\right) || \mathbb{P}\left(\theta | y\right)\right) = \operatorname*{argmin}_{\eta} \mathbb{E}_{\mathcal{N}\left(z\right)}\left[f(z | \eta)\right]$$

for a cleverly constructed, automatically-differentiable  $\eta\mapsto f(z|\eta)$ .

### Black box variational Bayes

"Black box variational Bayes" (BBVI) is a set of techniques for quickly and automatically approximating Bayesian posteriors using optimization. I'll consider "mean field automatic differentiation variational inference" (ADVI).

Let  $\theta$  denote model parameters and y some data and the joint generating distribution be  $\mathbb{P}(\theta,y) = \mathbb{P}(y|\theta)\mathbb{P}(\theta)$ . Let  $\mathbb{Q}(\theta|\eta)$  be a family of candidate approximate posteriors, here taken to be independent normals.

ADVI aims to find

$$\overset{*}{\eta} := \operatorname*{argmin}_{\eta} \operatorname{KL} \left( \mathbb{Q} \left( \theta | \eta \right) || \mathbb{P} \left( \theta | y \right) \right) = \operatorname*{argmin}_{\eta} \mathbb{E}_{\mathcal{N}(z)} \left[ f(z | \eta) \right]$$

for a cleverly constructed, automatically-differentiable  $\eta \mapsto f(z|\eta)$ .

Unfortunately,  $\mathbb{E}_{\mathcal{N}(z)}[f(z|\eta)]$  is typically intractable. So ADVI uses stochastic gradient (SG). The leads to the following problems:

- You have to tune the step size carefully
- You can't assess convergence directly
- You can't compute sensitivity, so you can't use linear response covariances.

 $\Rightarrow$  Optimization is slow and imprecise, and the posterior uncertainty is no good. Not so black box actually!

We propose a simple alternative to SG that resolves these problems (sometimes).

Suppse you want to minimize an objective function of the form

$$\mathring{\eta} := \operatorname*{argmin}_{\eta} \mathbb{E}_{\mathbb{P}(z)} \left[ f(z|\eta) \right] := \operatorname*{argmin}_{\eta} \ell(\eta),$$

where  $\mathbb{P}\left(z\right)$  is known, but the expectation is not available in closed form.

Suppse you want to minimize an objective function of the form

$$\mathring{\eta} := \operatorname*{argmin}_{\eta} \mathbb{E}_{\mathbb{P}(z)} \left[ f(z|\eta) \right] := \operatorname*{argmin}_{\eta} \ell(\eta),$$

where  $\mathbb{P}(z)$  is known, but the expectation is not available in closed form.

When does this happen?

- Black box variational inference
- Stochastic control (e.g. you have a factory, and supply and demand are random)

Suppse you want to minimize an objective function of the form

$$\mathring{\eta} := \operatorname*{argmin}_{\eta} \mathbb{E}_{\mathbb{P}(z)} \left[ f(z|\eta) \right] := \operatorname*{argmin}_{\eta} \ell(\eta),$$

where  $\mathbb{P}(z)$  is known, but the expectation is not available in closed form.

When does this happen?

- Black box variational inference
- Stochastic control (e.g. you have a factory, and supply and demand are random)

What can you do? There are two options, both using the Monte Carlo (MC) estimate

$$\hat{\ell}(\eta) := \frac{1}{N} \sum_{n=1}^{N} f(z_n | \eta) \approx \ell(\eta).$$

Suppse you want to minimize an objective function of the form

$$\mathring{\eta} := \underset{\eta}{\operatorname{argmin}} \mathbb{E}_{\mathbb{P}(z)} \left[ f(z|\eta) \right] := \underset{\eta}{\operatorname{argmin}} \ell(\eta),$$

where  $\mathbb{P}(z)$  is known, but the expectation is not available in closed form.

When does this happen?

- Black box variational inference
- Stochastic control (e.g. you have a factory, and supply and demand are random)

What can you do? There are two options, both using the Monte Carlo (MC) estimate

$$\hat{\ell}(\eta) := \frac{1}{N} \sum_{n=1}^{N} f(z_n | \eta) \approx \ell(\eta).$$

- Stochastic gradient (SG)
  - Update with  $\eta^i = \eta^{i-1} \rho \nabla_{\eta} \hat{\ell}(\eta)$  for some step size  $\rho$  (new  $z_n$  every step)
  - · Approximately minimizes the exact objective

Suppse you want to minimize an objective function of the form

$$\mathring{\eta} := \operatorname*{argmin}_{\eta} \mathbb{E}_{\mathbb{P}(z)} \left[ f(z|\eta) \right] := \operatorname*{argmin}_{\eta} \ell(\eta),$$

where  $\mathbb{P}(z)$  is known, but the expectation is not available in closed form.

When does this happen?

- Black box variational inference
- Stochastic control (e.g. you have a factory, and supply and demand are random)

What can you do? There are two options, both using the Monte Carlo (MC) estimate

$$\hat{\ell}(\eta) := \frac{1}{N} \sum_{n=1}^{N} f(z_n | \eta) \approx \ell(\eta).$$

- Stochastic gradient (SG)
  - Update with  $\eta^i = \eta^{i-1} \rho \nabla_{\eta} \hat{\ell}(\eta)$  for some step size  $\rho$  (new  $z_n$  every step)
  - Approximately minimizes the exact objective
- Sample average approximation (SAA)
  - Find  $\hat{\eta} := \operatorname{argmin}_{\eta} \hat{\ell}(\eta)$  for fixed  $z_n$
  - Exactly minimizes approximate objective

Suppse you want to minimize an objective function of the form

$$\mathring{\eta} := \operatorname*{argmin}_{\eta} \mathbb{E}_{\mathbb{P}(z)} \left[ f(z|\eta) \right] := \operatorname*{argmin}_{\eta} \ell(\eta),$$

where  $\mathbb{P}(z)$  is known, but the expectation is not available in closed form.

When does this happen?

- Black box variational inference
- Stochastic control (e.g. you have a factory, and supply and demand are random)

What can you do? There are two options, both using the Monte Carlo (MC) estimate

$$\hat{\ell}(\eta) := \frac{1}{N} \sum_{n=1}^{N} f(z_n | \eta) \approx \ell(\eta).$$

- Stochastic gradient (SG)
  - Update with  $\eta^i = \eta^{i-1} \rho \nabla_{\eta} \hat{\ell}(\eta)$  for some step size  $\rho$  (new  $z_n$  every step)
  - · Approximately minimizes the exact objective
- Sample average approximation (SAA)
  - Find  $\hat{\eta} := \operatorname{argmin}_{\eta} \hat{\ell}(\eta)$  for fixed  $z_n$
  - Exactly minimizes approximate objective

Which is better? In general, it depends.

As far as we can tell, the BBVI literature has only ever considered SG.

Sample average approximation (SAA)

- Find  $\hat{\eta} := \operatorname{argmin}_{\eta} \hat{\ell}(\eta)$
- $\bullet$  Fixed  $z_n$  for whole procedure
- Exactly minimizes approximate objective

Stochastic gradient (SG)

- $\eta^i = \eta^{i-1} \rho \nabla_{\eta} \hat{\ell}(\eta)$
- New z<sub>n</sub> every step
- Approximately minimizes the exact objective

Sample average approximation (SAA)

- Find  $\hat{\eta} := \operatorname{argmin}_{\eta} \hat{\ell}(\eta)$
- $\bullet$  Fixed  $z_n$  for whole procedure
- Exactly minimizes approximate objective

#### Advantages:

- Can use fast off-the-shelf second-order optimization (great for poorly-conditioned problems)
- Can evaluate the objective function exactly to check for convergence
- Can compute sensitivity (linear response covariances ⇒ more accurate posterior covariances for mean field approximations)

Stochastic gradient (SG)

- $\eta^i = \eta^{i-1} \rho \nabla_{\eta} \hat{\ell}(\eta)$
- New z<sub>n</sub> every step
- Approximately minimizes the exact objective

Sample average approximation (SAA)

- Find  $\hat{\eta} := \operatorname{argmin}_{\eta} \hat{\ell}(\eta)$
- $\bullet$  Fixed  $z_n$  for whole procedure
- Exactly minimizes approximate objective

### Advantages:

- Can use fast off-the-shelf second-order optimization (great for poorly-conditioned problems)
- Can evaluate the objective function exactly to check for convergence
- Can compute sensitivity (linear response covariances ⇒ more accurate posterior covariances for mean field approximations)

Stochastic gradient (SG)

- $\eta^i = \eta^{i-1} \rho \nabla_{\eta} \hat{\ell}(\eta)$
- New z<sub>n</sub> every step
- Approximately minimizes the exact objective

### Advantages:

 Uses each draw z<sub>n</sub> only once (for a single gradient step)

Sample average approximation (SAA)

- Find  $\hat{\eta} := \operatorname{argmin}_{\eta} \hat{\ell}(\eta)$
- $\bullet$  Fixed  $z_n$  for whole procedure
- Exactly minimizes approximate objective

#### Advantages:

- Can use fast off-the-shelf second-order optimization (great for poorly-conditioned problems)
- Can evaluate the objective function exactly to check for convergence
- Can compute sensitivity (linear response covariances ⇒ more accurate posterior covariances for mean field approximations)

Stochastic gradient (SG)

- $\eta^i = \eta^{i-1} \rho \nabla_{\eta} \hat{\ell}(\eta)$
- New z<sub>n</sub> every step
- Approximately minimizes the exact objective

#### Advantages:

 Uses each draw z<sub>n</sub> only once (for a single gradient step)

This is actually a big one! Because if  $\eta \in \mathbb{R}^D$ , in general, both SG and SAA have accuracy  $(D/N)^{-1/2}$ , where N is the *total* number of draws of  $z_n$  used.

SAA uses each draw at each step of optimization. SG uses each draw once. ⇒ In general, SG is much more efficient in high dimensions!

Sample average approximation (SAA)

- Find  $\hat{\eta} := \operatorname{argmin}_{\eta} \hat{\ell}(\eta)$
- $\bullet$  Fixed  $z_n$  for whole procedure
- Exactly minimizes approximate objective

#### Advantages:

- Can use fast off-the-shelf second-order optimization (great for poorly-conditioned problems)
- Can evaluate the objective function exactly to check for convergence
- Can compute sensitivity (linear response covariances ⇒ more accurate posterior covariances for mean field approximations)

Stochastic gradient (SG)

- $\eta^i = \eta^{i-1} \rho \nabla_{\eta} \hat{\ell}(\eta)$
- New z<sub>n</sub> every step
- Approximately minimizes the exact objective

#### Advantages:

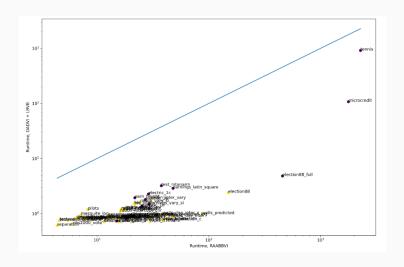
 Uses each draw z<sub>n</sub> only once (for a single gradient step)

This is actually a big one! Because if  $\eta \in \mathbb{R}^D$ , in general, both SG and SAA have accuracy  $(D/N)^{-1/2}$ , where N is the *total* number of draws of  $z_n$  used.

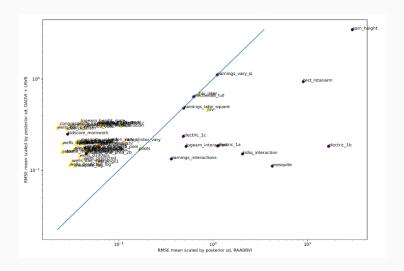
SAA uses each draw at each step of optimization. SG uses each draw once.  $\Rightarrow$  In general, SG is much more efficient in high dimensions!

**Theorem (us).** If  $\log \mathbb{P}(\theta, y)$  is high dimensional due to a large number of "local" variables, then the accuracy is  $(\log D/N)^{-1/2}$ , rendering SAA feasible.

# **Experimental results: Runtime**



# **Experimental results: Means**



### **Experimental results: Standard deviations**

